HANAMI

Deliverable D1.8

Follow-up of the scientific collaborations with Japanese partners-3

Funded by the European Union

EuroHPC Joint Undertaking

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D1.8 - Follow-up of the scientific collaborations with Japanese partners-3

Project Title	**Hpc AlliaNce for Applications and supercoMputing Innovation: the Europe - Japan collaboration**
Project Ref	EuroHPC International Cooperation (HORIZON-EUROHPC-JU-2022-INCO-04)
Project Acronym	HANAMI
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Topic	HORIZON JU Research and Innovation Actions
Starting Date of Project	2024-03-01
Ending Date of Project	2028-02-28
Duration of the Project	36 months
Website	http://hanami-project.com/

Work Package	**1**
Task	1.8
Lead Authors	France Boillod-Cerneux (CEA) Edouard Audit (CEA) Christophe Calvin (CEA)
Contributors	All members of HANAMI WP4, WP5 and WP6
Peer Reviewers	Pablo Ordejon (ICN2) Edoardo Di Napoli (FZJ)
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Due Date	31.08.25
Submission Date	21.08.25

D1.8 - Follow-up of the scientific collaborations with Japanese partners-3

Dissemination Level

X	PU: Public
	SEN: Sensitive – limited under the conditions of the Grant Agreement
	EU-RES. Classified Information: RESTREINT UE (Commission Decision 2005/444/EC)
	EU-CON. Classified Information: CONFIDENTIEL UE (Commission Decision 2005/444/EC)
	EU-SEC. Classified Information: SECRET UE (Commission Decision 2005/444/EC)

D1.7 - Follow-up of the scientific collaborations with Japanese partners-3

Revision	Date	Editors	Comments
1.0	01.07.25	France Boillod-Cerneux (CEA)	Template to retrieve the HANAMI work packages information.
1.1	19.08.25	HANAMI members	Providing inputs for all work packages
2.0	21.08.25	France Boillod-Cerneux (CEA)	Gathering the work packages presentations and consolidating the deliverable.

D1.8 Executive Summary

This deliverable focuses on the follow-up of HANAMI collaboration with Japanese partners.

In the following presentation, we present HANAMI work packages in strong interaction with HANAMI Japanese partners and details ongoing and future actions, designed and led jointly by European and Japanese researchers involved within HANAMI.

This document will serve as a basis to highlight HANAMI collaboration with Japan, and will be regularly updated, leading to respectively D1.6 (submitted on month 6, in August 2024), D1.7, D1.8 (the current deliverable), and later, D1.9 and D1.10.

D1.8 Outlines

- **WP4 – Application development for the climate and weather modelling community**
- **WP5 – Biomedical application co-development to address societal challenges**
- **WP6 – HPC for future materials design**

WP4

Application development for the climate and weather modelling community

WP4 objectives and presentation

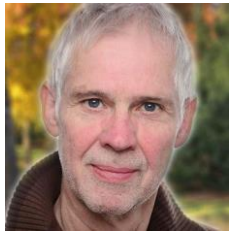
WP4 Application development for the climate and weather modeling community

- Connect Japanese and European efforts and expertise to improve the performance of codes for weather and climate simulations
  - Assess and improve the computational performance, replicability and accuracy of our European Earth System Models as a whole, tested on European and Japanese HPC platforms
  - Optimize, port and test European models on Japanese supercomputers
  - Incorporate Japanese weather and climate codes into our European benchmarks to be used on EuroHPC platforms

WP4 Application development for the climate and weather modelling community

Work package leaders

Mario Acosta



Joachim Biercamp

HANAMI members

Barcelona Supercomputing Center
Centro Nacional de Supercomputación

DKRZ
Deutsches Klimarechenzentrum

CSC

ECMWF

University of Warsaw

- Project 1: Replicability and skill of earth system models - Workflow and Interface
  - Task 4.1: Model assessment for earth system models and the integration through the workflow manager Autosubmit
- Project 2: Optimize, port and test European and Japan weather and climate codes
  - Task 4.2: High-Performance Climate and Weather benchmark
  - Task 4.3: The University of Warsaw Lagrangian Cloud Model (UWLCM)

HANAMI participants

EVIDEN

RIKEN

東京大学 先端科学技術研究センター
Research Center for Advanced Science and Technology
The University of Tokyo

National Institute for Environmental Studies

WP4 Application development for the climate and weather modelling community – **research team**

Mario Acosta

Kai Keller

Thomas Ludwig

Marta Alerany

Mohamed Wahib

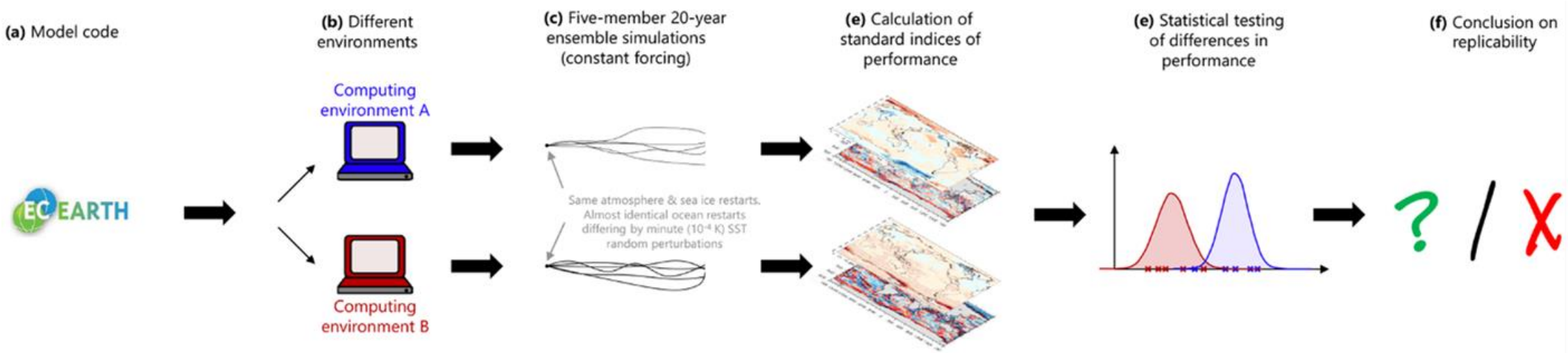
Leo Arriola

Hisashi Yashiro

T4.1: Model assessment for earth system models and the integration through the workflow manager Autosubmit

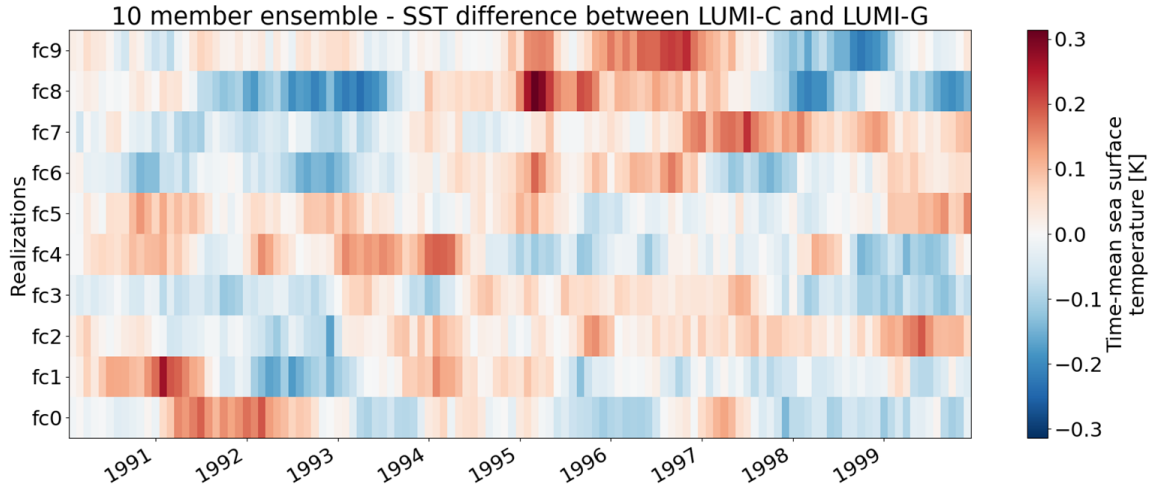
- The team develops a workflow (orchestrator and monitor in a self-contained application) for testing three aspects of earth system models (ESM): 1. replicability, 2. projection skill, and 3. computational performance.
- Those methodologies are combined inside a single workflow with a generic interface applicable to any weather and climate model and accessible on any cluster.

Earth System Model (ESM) performance assessment

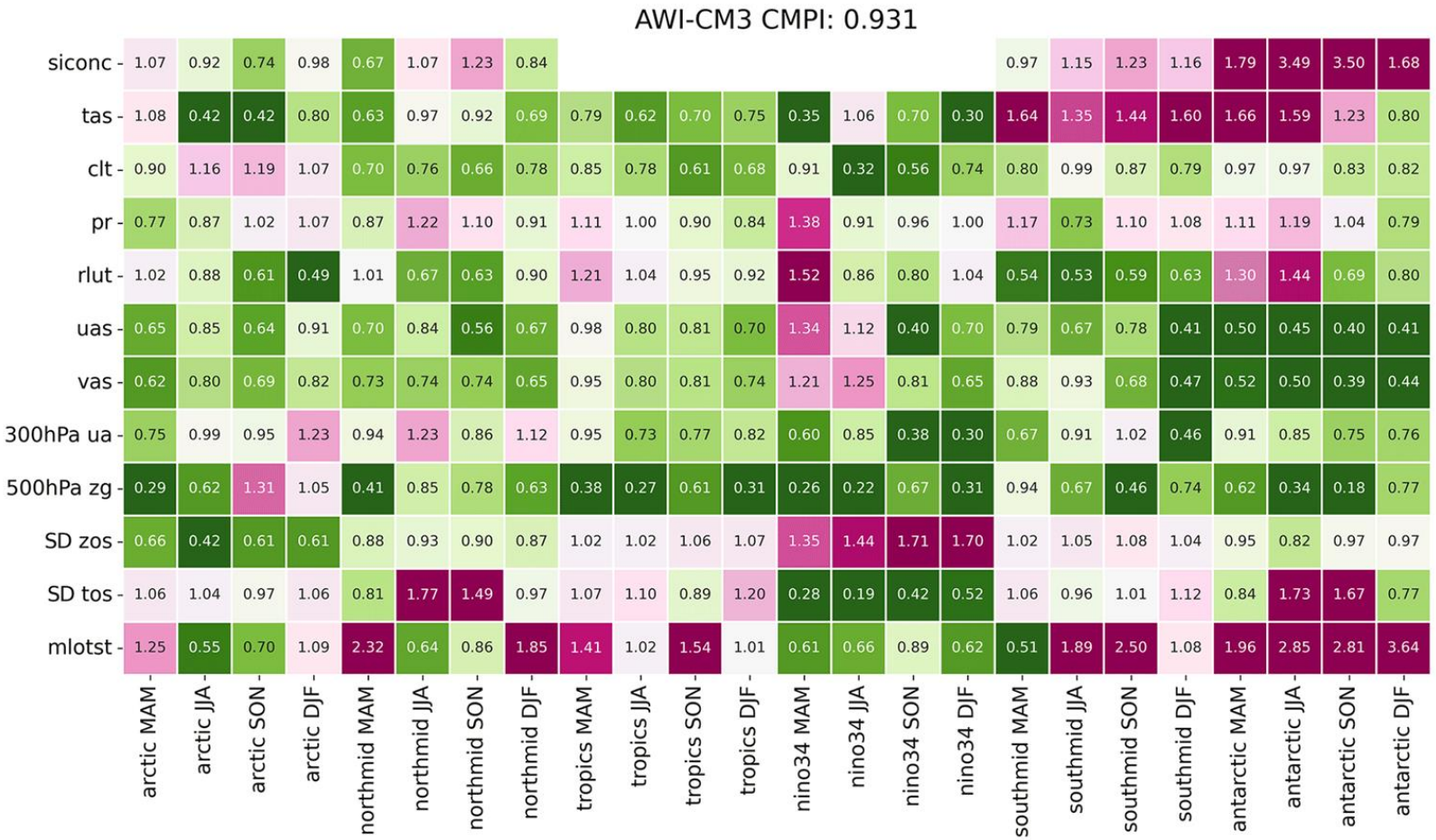


Massonnet, F., Ménégoz, M., Acosta, M., Yepes-Arbós, X., Exarchou, E., & Doblas-Reyes, F. J. (2020). **Replicability of the EC-Earth3 Earth system model under a change in computing environment.** Geoscientific Model Development, 13(3), 1165–1178. https://doi.org/10.5194/gmd-13-1165-2020

- ***Testing three aspects of ESMs***
  - ***I. Replicability***
  - ***II. Projection skill***
  - ***III. Computational performance***



Earth System Model (ESM) performance assessment



Testing three aspects of ESMs

I. ***Replicability***
II. ***Projection skill***
III. ***Computational performance***

Reichler & Kim indices a.k.a. Performance scores

Streffing, J., Sidorenko, D., Semmler, T., Zampieri, L., Scholz, P., Andrés-Martínez, M., Koldunov, N., Rackow, T., Kjellsson, J., Goessling, H., Athanase, M., Wang, Q., Hegewald, J., Sein, D. V., Mu, L., Fladrich, U., Barbi, D., Gierz, P., Danilov, S., … Jung, T. (2022). **AWI-CM3 coupled climate model: Description and evaluation experiments for a prototype post-CMIP6 model.** Geoscientific Model Development, 15(16), 6399–6427. https://doi.org/10.5194/gmd-15-6399-2022

Earth System Model (ESM) performance assessment

Metric	Description
Simulation Year Per Day (SYPD)	Simulated years per day in a 24 h period, collected by timing a segment of a production run of usually one year.
Core-hours Per year Simulated (CHSY)	Simulated years produced with respect to the number of parallel resources used
Complexity (Cmpx)	number of prognostic variables per component
Actual SYPD (ASYPD)	how queue time and interruptions affect the complete experiment duration
Parallelization (Paral)	total number of cores allocated for the run
Energy Cost Per Year (JPSY)	Energy in Joules needed per year of simulation
Memory Bloat (Mem B)	ratio between actual and ideal memory size
Data Output Cost (DO)	time and resources used for performing I/O. The value is given as the percentage added to the simulation without outputs. For example, 1.05 means that DO is 5%.
Data Intensity (DI)	amount of data produced in GB per compute-hour
Coupling Cost (Coup C)	time and resources used in the execution of the coupling algorithm as well as load imbalance among model components. The value is given as the percentage represented comparing to the simulation of the components without coupling. For example, 0.05 means that Coup. C. is 5%.

- ***Testing three aspects of ESMs***
  - *I.* ***Replicability***
  - *II.* ***Projection skill***
  - *III.* ***Computational performance***

Balaji, V., Maisonnave, E., Zadeh, N., Lawrence, B. N., Biercamp, J., Fladrich, U., Aloisio, G., Benson, R., Caubel, A., Durachta, J., Foujols, M.-A., Lister, G., Mocavero, S., Underwood, S., & Wright, G. (2017). **CPMIP: Measurements of real computational performance of Earth system models in CMIP6.** Geoscientific Model Development, 10(1), 19–34. https://doi.org/10.5194/gmd-10-19-2017

project outcome

We aim to deploy the new workflow on European and Japanese supercomputers and to develop a sustainable collaboration connecting Japanese and European efforts on weather and climate model development.

A collaborative effort in porting European and Japanese models to the workflow and assessing their replicability, projection skill, and performance on European and Japanese supercomputers.

WP4 Application development for the climate and weather modelling community – **research team**


Joachim Biercamp


Miguel Castrillo


Leopekka Saraste


Juhana Lankinen


Peter Duben


Chihiro Kodama


Samuel Hatfield


Erwan Raffin


Hisashi Yashiro

T4.2: High-Performance Climate and Weather benchmark

- CMake-based framework
  - to build all models and their dependencies
  - to bench all models with their test cases
  - to report the results
- Current models available
  - ICON - Ocean and Atmosphere
  - NEMO (Ocean)
  - Mini-applications (dwarfs):
    - ecRad, ecTrans. Dwarf-P-CloudSC

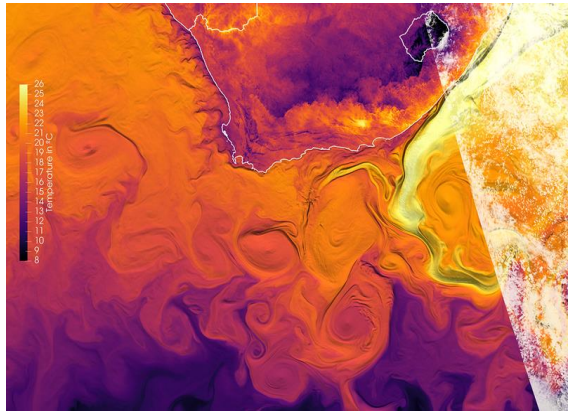
- Verification procedures for automatic correctness checking
- 3 test-cases per model of increasing size (small, medium, big)
- Automatic performance metrics extraction, e.g. time to solution

- SPACK recipes to build the models
- A way to use already installed models

- Uses gitlab CI
- Has been pushed to CASTIEL2 gitlab server

HANAMI aims to extend to new HW architectures, include Japanese Components (NICAM), measure, document, learn, improve

World leading simulation codes



Tokyo, November 20, 2020

Japanese Group Performs Largest Ever Meteo-rological Calculation on Supercomputer Fugaku

Collaboration of supercomputer, simulation, and data science opens up Future Weather Forecast

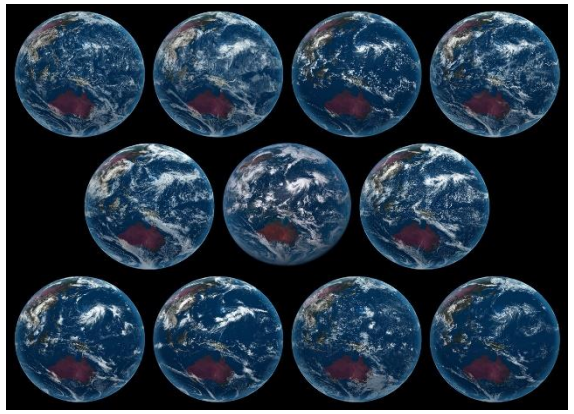
(National Institute for Environmental Studies,RIKEN,Fujitsu Limited,Metro, Inc.,Atmosphere and Ocean Research Institute, The University of Tokyo)

Hamburg, 6. Oct 2022

Technical milestone reached: global Earth system simulations with 1.2 km resolution

A new chapter in Earth System Modelling that has been a dream for climate scientists and seemed very distant for ages.

Max Planck Institute for Meteorology (MPI-M)



Scientific Assessment

DYAMOND (DYnamics of the Atmospheric general circulation Modeled On Non-hydrostatic Domains)

A framework for the intercomparison of global storm-resolving models initiated by

Max Planck Institute for Meteorology (MPI-M, Bjorn Stevens) and University of Tokyo (Masaki Satoh).

DYAMOND demonstrated the enormous potential of this type of models which need exascale capabilities to be operationally capitalized

(Make the “Palmer-Turing-Test”: Which one is the satellite image?)

HPCW

Technical Assessment and co-design ? HANAMI T4.2

HPCW: The High Performance Weather and Climate Benchmark

- set of relevant and realistic, near-operational weather and climate workloads
- targeted to exa-scale
- ideal for co-design and performance assessment of SW and HW

WP4 Application development for the climate and weather modelling community – **research team**

Hanna Pawlowska Piotr Dziekan Sin-Ichiro Shima Seiya Nishizawa Hirofumi Tomita





T4.3: The University of Warsaw Lagrangian Cloud Model (UWLCM)

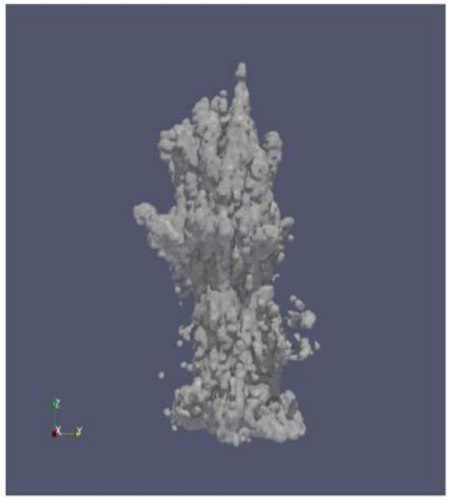
Optimize UWLCM code (cloud model using the large-eddy simulation aproximation) for modern European and Japanese computing clusters.

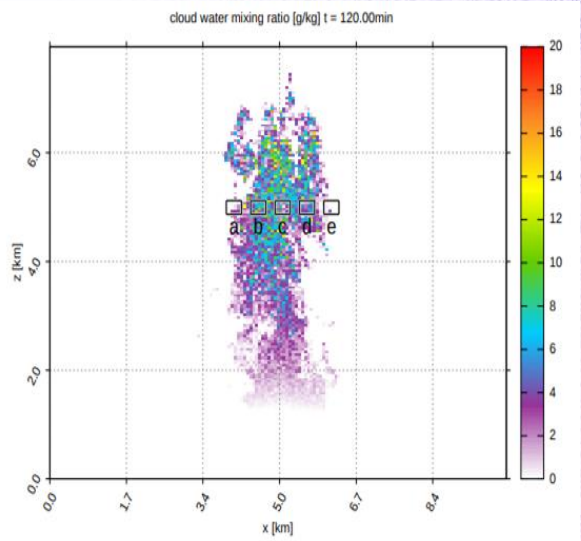
The University of Warsaw Lagrangian Cloud Model (UWLCM)

UNIVERSITY OF WARSAW

Numerical simulations of clouds using the large-eddy simulation (LES) approximation

- Typical LES resolution is of the order of tens of meters.
- Lagrangian microphysics computed on GPUs (or CPUs)
- Useful for developing/improving realistic cloud microphysics parametrization for coarser resolution models

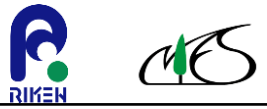




The proposed work will improve the UWCLM model, but will also help develop techniques for optimizing CPU+GPU codes in general, and for optimizing cloud models that use Lagrangian cloud microphysics for European and Japanese

WP4 ongoing actions

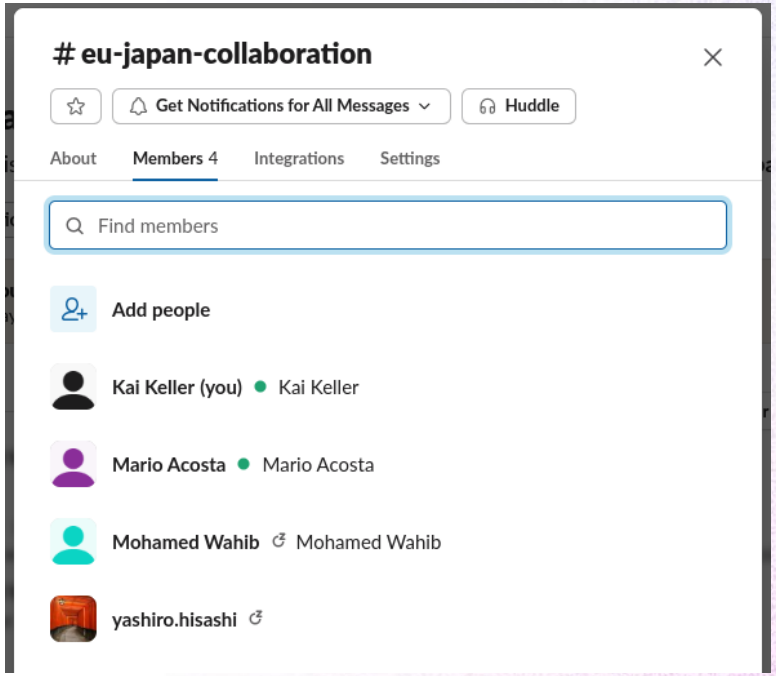
WP4T4.1 Replicability and skill of earth system models - Workflow and Interface

		workflow manager Autosubmit
M6 01.08.2024 until M18 01.09.2025		Develop the model assessment workflow addressing the requirements of ESMs from the European and Japanese partners
		Deploy Autosubmit and the proposed workflow on Marenostrum 5, LUMI, and Fugaku.
		-
		Porting Japanese models to the workflow and assessing their replicability, projection skill, and performance on heterogeneous architectures

M4.1	Several collaborative interactions in place (workshops and meetings)	M06 - 06.2024
R4.1	**Autosubmit workflow on Marenostrum5, LUMI and Fugaku (interim version)**	**M18 – 08.2025**
R4.2	Autosubmit workflow on Marenostrum5, LUMI and Fugaku (final version)	M33 – 12.2026

WP4T4.1 Replicability and skill of earth system models - Workflow and Interface

- Close collaboration with Hisashi Yashiro (NIES) and Chihiro Kodama (JAMSTEC)
- Joint workflow development for NICOCO in Autosubmit
- Submitted two joint proposals:
  - Fugaku general access (rejected, in the top 20%, resubmission in May for October access)
  - JHPCN international project
    - Miyabi access
    - Travel and conference funding
- Long stay of Marta Alerany at JAMSTEC in May 2025 (6 weeks)
- Marta Alerany and Kai Keller attended the JpGU meeting in May in Tokyo
  - session on high resolution modeling, convener: Hisashi Yashiro



WP4T4.1 Replicability and skill of earth system models - Workflow and Interface

Joint session proposal accepted at the AOGS annual meeting 2025 (AS36 - Weather and Climate Studies with High Resolution Earth System Models and High Performance Computing)

- **Supercomputers access**
  - Access granted for WP4P1 European team to Fugaku through HPCI access – duration: 05.2024 until 04.2025
    - Maximum of computing hours: 40000 nh
  - **The team has now access to Fugaku thanks to the EuroHPC-R-CCS Letter of Intent**

- Development access on Marenostrum5 - duration: 10.2024 until 09.2025
  - Maximum computing hours (node hours): 4000

  - Access granted for WP4P1 Japanese researchers to LUMI through bilateral MoU CSC and RIKEN/R-CCS – duration: 05.2024 until 04.2026
  - Maximum of computing hours: 40000

WP4T4.2 Optimize, port and test European and Japan weather and climate codes

M6 01.08.2024 until M18 01.09.2025	DKRZ	Extending the existing test cases in HPCW; assistance with implementation of NICAM-DC into HPCW; general maintenance and preparations for first open-source release of HPCW
	BSC	Preparing HPCW for MN5 deployment
	ECMWF	Worked on extending NICAM-DC benchmark in HPCW to higher resolution test cases, began investigation of integrating Japanese SCALE model in to HPCW to complement NICAM-DC
	CSC	Began building of and preparations for running the HPCW codes on LUMI

M4.1	Several collaborative interactions in place (workshops and meetings)	M06 - 06.2024
R4.3	**Report on detailed work plan for extension of HPCW** **Report on extensions made to the HPCW benchmarks including results and conclusions**	**M18 – 08.2025**
R4.4	Report on detailed work plan for extension of HPCW Report on extensions made to the HPCW benchmarks including results and conclusions	M33 – 12.2026

WP4T4.2 Optimize, port and test European and Japan weather and climate codes

- Monthly WP4-wide meetings (including Japanese partners)
- Coordination with Japanese partners on Japanese HPCW components via email (e.g. NICAM)

- **Supercomputers access**
  - Access granted to Fugaku for HPCW porting via Fugaku Trial Access – duration: 02.25 until 08.25
    - Maximum of computing hours: 50000 nh
  - **The team has now access to Fugaku thanks to the EuroHPC-R-CCS Letter of Intent**

- **Visits in 2025**
  - 2-4 week trip to Hisashi Yashiro, NIES (Tsukuba, Japan) for Samuel Hatfield and Niclas Schroeter under discussion, to take place in January 2025
  - Joint session proposal at JpGU, May 2025 with Hirofumi Tomita (R-CCS), Hisashi Yashiro (NIES), and Chihiro Kodama (JAMSTEC)

WP4T4.3 Optimize, port and test European and Japan weather and climate codes

T4.3 - The University of Warsaw Lagrangian Cloud Model		
M6 01.08.2024 until 01.09.2025	UNIVERSITY OF WARSAW	Interactions with WP4 members during online meetings and with the entire Hanami team during HLS. WP4T4.3 realization is to start in M18. Visits to Japan planned for 09.2025.
	UNIVERSITY OF HYOGO MMIV / RIKEN	Interactions with WP4 members during online meetings and with the entire Hanami team during HLS. WP4T4.3 realization is to start in M18. Visits to Japan planned for 09.2025.

M4.1	Several collaborative interactions in place (workshops and meetings)	M06 - 06.2024
R4.5	The scope of this deliverable will be to report activities for UWLCM	M33 – 12.2026

WP4T4.3 Optimize, port and test European and Japan weather and climate codes

- Monthly meetings with Japanese researchers
  - Regular exchanges on ICON
  - UWLCM: exchanges and information on framework

- Supercomputers access
  - Asked for LUMI and FUGAKU access via the Hanami call
  - **The team has now access to Fugaku thanks to the EuroHPC-R-CCS Letter of Intent**

- Visits in 2025
  - UW team is travelling in Japan in September 2025 to meet their Japanese coworkers
    - Visited laboratory: University of Hyogo, Kobe, Japan

WP5

Biomedical application co-development to address societal challenges

WP5 objectives and presentation

WP5 Biomedical application co-development to address societal challenges

- Advancing molecular life sciences computing by joint development of Exascale-focused algorithms
  - major simulation codes developed both in EuroHPC (GROMACS) and at RIKEN (GENESIS),
  - fast-multipole electrostatics,
  - bridging simulations and AI by implementing support for neural network-based nonbonded potentials.

- Pursing data-driven life science by developing new HPC models to integrate experimental data such as cryoEM/ET, single-molecule FRET and high-speed AFM in molecular modeling and simulations.

- Developing techniques to perform whole-minimal-cell simulations with hundreds of millions of coarse-grained particles.

- Developing a comprehensive pipeline for cancer genome analysis in the context of the International Cancer Genome Consortium and European 1+ million genomes based on recommendations and network of standards in the Global Alliance for Genomic Health.

- Implementing a pipeline for simulation of tumor evolution based on individual genomic information within the PhysiBOSS cell-scale simulation environment.

- Combining large-scale computational fluid dynamics simulations with machine learning techniques for an improved analysis of respiratory diseases and virus particle spread in indoor scenarios

WP5 Biomedical application co-development to address societal challenges

Work package leaders

Erik Lindahl

Alfonso Valencia

HANAMI members

KTH VETENSKAP OCH KONST

BSC Barcelona Supercomputing Center Centro Nacional de Supercomputación

CSC

JÜLICH Forschungszentrum

HANAMI participants

RIKEN

R-CCS

RIKEN BDR

東京工業大学 Tokyo Institute of Technology

九州大学 KYUSHU UNIVERSITY

東京大学 THE UNIVERSITY OF TOKYO

NAGOYA UNIVERSITY

university of groningen

Kobe University Graduate School of System Informatics
Kobe University Department of Computer Science and Systems Engineering

東京大学 先端科学技術研究センター
Research Center for Advanced Science and Technology
The University of Tokyo

WP5 Biomedical application co-development to address societal challenges

- WP5 – P1: Exascale electrostatics & machine learning to enable molecular dynamics of cell-size systems
  - Extend existing collaborations on software and hardware in molecular dynamics simulation into long-term coordinated development of the two major-impact codes GROMACS (EU) and GENESIS (RIKEN),
  - Coordination with the simulation hardware developed in the RIKEN MD-GRAPE project
  - The two codebases GENESIS and GROMACS complement each other
    - both codes used as benchmarks and optimization targets in the post-Fugaku projects
    - unique codesign opportunity for both the European and Japanese

WP5 Biomedical application co-development to address societal challenges

- WP5 – P2: Development of genome analysis pipelines for Personalized Medicine
  - Provide mechanistic models for individual patients reflecting their differential genomic composition and response to treatments
  - Interpret mechanistic models with field-experts to identify potential treatments and/or associated signatures
  - Contribute to the technical development of practical implementations that facilitate the work of clinicians and genome scientists, ultimately leading to better and more tailored treatment strategies for cancer patients

WP5 Biomedical application co-development to address societal challenges

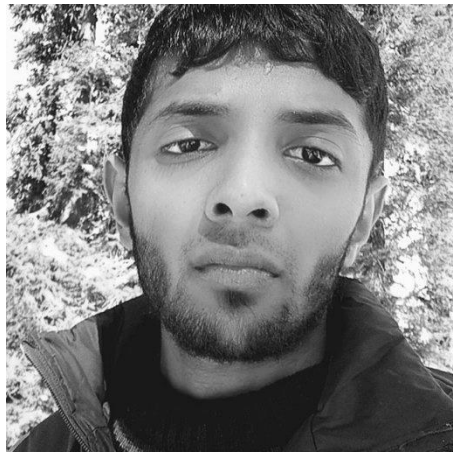
- WP5 – P3: Personalized Medicine on Macroscopic Level: Respiratory Flows and Infection Risk Analyses
  - Develop a pipeline for AI-assisted automated large-scale computational fluid dynamics (CFD) simulations to analyze respiratory diseases
  - Use AI-methods to accelerate CFD simulations
  - Provide an AI-assisted automated surgery tool to surgeons as a demonstrator
  - Develop a tool for assessing the risk of exhaled infectious (virus) in indoor scenarios
  - All implementations complement missing elements in either the m-AIA (EU) or the CUBE (Japan) CFD solvers
  - AI methods are jointly developed with the Japanese partners

WP5 Biomedical application co-development to address societal challenges – **research team**

Prof. Berk Hess

Szilárd Páll

Dr. Muhammad Sadiq



Prof. Erik Lindahl

Assoc. Prof Rio Yokota

T5.1: ExaFMM - solving the scaling problem for electrostatic interactions

WP5 Biomedical application co-development to address societal challenges – **research team**

Prof. Erik Lindahl

Dr. Alessandra Villa

Prof. Berk Hess

Dr. Muhammad Sadiq

Prof. Yuji Sugita

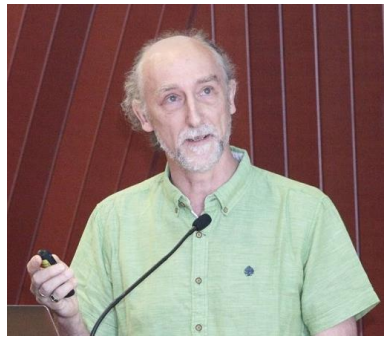
Dr. Mohamad Wahib

Prof. Makoto Taiji

Prof. Florence Tama

T5.2: Data-driven biomolecular modeling & simulation

WP5 Biomedical application co-development to address societal challenges – **research team**



Alfonso Valencia

Tommi Nyrönen

EU Japan

Elisa Domínguez-Hüttinger
(PRIMe - Osaka University)

Mariko Okada
(Osaka University)

T5.4: Tumour evolution simulation pipelines

WP5 Biomedical application co-development to address societal challenges – **research team**

FZJ

Dr. Andreas Lintermann

Dr. Mario Rüttgers

(Until 01.01.2025)

Alex (Oleksandr) Krochak

(From 01.01.2025)

RIKEN-CCS

Prof. Makoto Tsubokura

Dr. Junya Onishi

T5.5: AI-assisted automated CFD pipelines and acceleration of CFD computations
T 5.6: AI-assisted surgery planning and risk assessment of exhaled infectious aerosols

WP5 ongoing actions

WP5P1 Exascale electrostatics & machine learning to enable molecular dynamics of cell-size systems

M1 01.03.2024 until M36 27.02.2027	KTH R-CCS	Explore FMM to enable both GROMACS and GENESIS to scale to hundreds of thousands of ranks
	KTH R-CCS	combine the world-leading EU-based molecular simulation code GROMACS with the world leading FFM package ExaFMM developed by Rio Yokota. Turns ExaFMM into a library that can be coupled efficiently to GROMACS Integrate the same code with GENESIS
	KTH R-CCS	Enable both longer simulation times for a given system size, as well as the ability to simulate extreme-scale systems such as entire cells with hundreds of millions of particles.

M5.1	**Several collaborative interactions in place such as visits and exchanges**	**M18 – 08.2025**
R5.1	Biomedical project setup roadmap	M06 - 06.2024

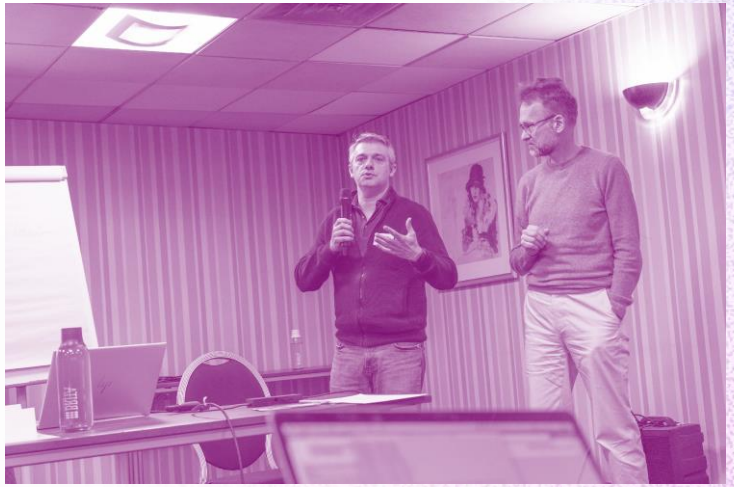
WP5P1 Exascale electrostatics & machine learning to enable molecular dynamics of cell-size systems

M1 01.03.2024 until M36 27.02.2027	KTH, R-CCS, RIKEN BDR	work on improving the support for neural network/deep learning potentials by integrating DeepMD and other packages into both GROMACS and GENESIS, Evaluate the possibility of directly implementing code to do the inference stage
	KTH, R-CCS, RIKEN BDR	Address the challenges with sensitivity to training domains, Investigate possibilities to use “delta-learning”, Apply neural networks as a correction
	KTH, R-CCS, Nagoya University, RIKEN BDR, Oxford	Develop new algorithms to combine this type of data Develop code to make it possible to restrain an ensemble of simulations Extend GROMACS to make it possible to perform coarse-grained molecular modeling of cellscale systems restrained with low-resolution experimental data

M5.1	Several collaborative interactions in place such as visits and exchanges	M18 – 08.2025
R5.2	Biomedical halftime report	M18 – 08.2025

WP5P1 Exascale electrostatics & machine learning to enable molecular dynamics of cell-size systems

- Active collaboration with Japanese researchers regarding Long-range electrostatics work
  - Zoom meetings are held after two to four weeks to share updates and coordinate efforts
  - Extensive RIKEN contributions to GROMACS SVE acceleration and regression testing on Fugaku hardware
  - Joint Exascale-target fast multipole implementation is actively ongoing with Prof. Rio Yokota
    - A shared repository is hosting code compatible with both GROMACS and ExaFMM
  - A joint publication is planned for the ongoing work related to the regularized fast multipole method
  - An interface between ExaFMM and GROMACS has been implemented and is ready for integration into GROMACS
- RIKEN-CCS GENESIS team has become involved in definitions of joint file formats and data exchange standards run by the EU teams



WP5P1 Exascale electrostatics & machine learning to enable molecular dynamics of cell-size systems

- Planned research visits:
  - Dr. Muhammad Sadiq visit in Tokyo Tech mid-to-late 2025 for joint ExaFMM work
  - Prof. Berk Hess visit to RIKEN & Tokyo Tech planned mid-to-late 2025 to finalize work
  - Prof. Erik Lindahl to visit RIKEN-CCS & RIKEN-BDR in Kobe both 2025 & 2026 to work on data-driven simulations and applications to large systems

- New AI4SCIENCE frameworks both in Sweden & Japan to focus on data-driven work and foundation models. Will pursue new collaborations with Profs. Yuji Sugita & Satoshi Matsuoka.

- Leverage: JST ASPIRE Call proposal – submitted on 04.2024
  - PI: Mohamed Wahib, RIKEN/R-CCS
  - Letter of support from HANAMI
  - Proposal under review.

WP5P1 Exascale electrostatics & machine learning to enable molecular dynamics of cell-size systems

- Codes WP5P1

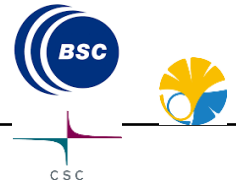
GROMACS	MARENOSTRUM 5, MELUXINA, KAROLINA, DISCOVERER, VEGA, DEUCALION, LEONARDO	Production, fully optimized.
	LUMI	Production, further HIP-specific optimization in progress
	Fugaku	Production, further SVE-specific optimization in progress
	JUPITER, JULES VERNE	Production will be supported day 1. New SVE-optimization in progress based on Fugaku work.

WP5P2 Development of genome analysis pipelines for Personalized Medicine

M1 01.03.2024 until M36 27.02.2027		genome analysis pipeline with variants for different type of genomic data
		use different type of genomic and clinical information including real data complemented with generated synthetic data
		modelling of the cohorts of synthetic data between the participating labs in Japan and Europe
		data sets analysed in the context of the information available in large cancer projects and repositories, including ICGC and others sources of genomic data at the single cell level, e.g., tissue specific single cell expression data recently published.

M5.1	Several collaborative interactions in place such as visits and exchanges	M18 – 08.2025
R5.3	Biomedical final results	M36 – 02.2027

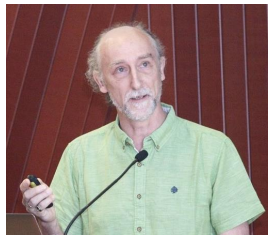
WP5P2 Development of genome analysis pipelines for Personalized Medicine

M1 01.03.2024 until M36 27.02.2027		Adaptation of the intracellular pathways to the patient specific data (mutations and gene expression levels) and the simulation of tumour evolution within the PhysiBoSS agent based component.
		integration of the genome analysis and simulation workflows and their adaptation to the operation in new hardware environments, with particular emphasis in new implementation adapted to GPU infrastructures
		produce pipelines that can be executed by non-experts without the need of further adaptations beside setting the input data and basic parameters

M5.1	Several collaborative interactions in place such as visits and exchanges	M18 – 08.2025
R5.4	Final report on scientific progress in molecular life science and personalized medicine, as well as updated long-term collaboration roadmap	M36 - 02.2027

WP5P2 Development of genome analysis pipelines for Personalized Medicine

- Monthly meetings with Japanese researchers
  - Evaluate synthetic data generation pipelines
    - How to integrate somatic alterations from real patients to improve synthetic data quality
    - Potential applications in Personalised Medicine and computational biology
  - Plan research visits
  - Coordinately organise workshops on HPC-simulations in biology
  - Explore opportunities for joint publications
  - Organise inter-center working teams



Alfonso Valencia (BSC)

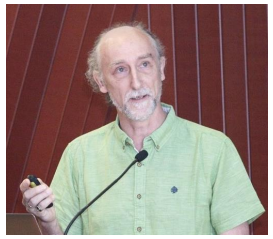
Tommi Nyrönen (CSC)

Mariko Okada (Osaka University)

Elisa Domínguez-Hüttinger (PRIMe - Osaka University)

WP5P2 Development of genome analysis pipelines for Personalized Medicine

- Monthly meetings with Japanese researchers
  - Identify grand challenges in Personalised Medicine requiring exascale capacities
    - Large-scale prediction of combinatorial drug treatments
    - Explore landscape of attractors in super complex molecular pathways
    - Integration of genome-scale metabolic networks in cellular simulations
    - Hero runs: From molecular features to whole organ simulations



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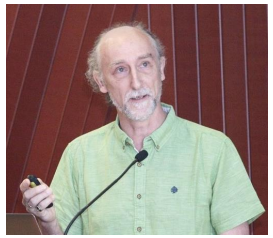
WP5P2 Development of genome analysis pipelines for Personalized Medicine

- Coordinate efforts for computationally benchmarking of genomic pipelines in European + Japanese HPC facilities
  - Comparative test in MN5-LUMI vs Fugaku
  - Evaluate parallel and distributed computing efficiency on…
    - Synthetic data generation pipelines
    - Tumour evolution multiscale simulations
  - Metrics
    - CPU time, memory consumption or I/O
    - Parallel and communication efficiency and computational scalability
    - Energy metrics



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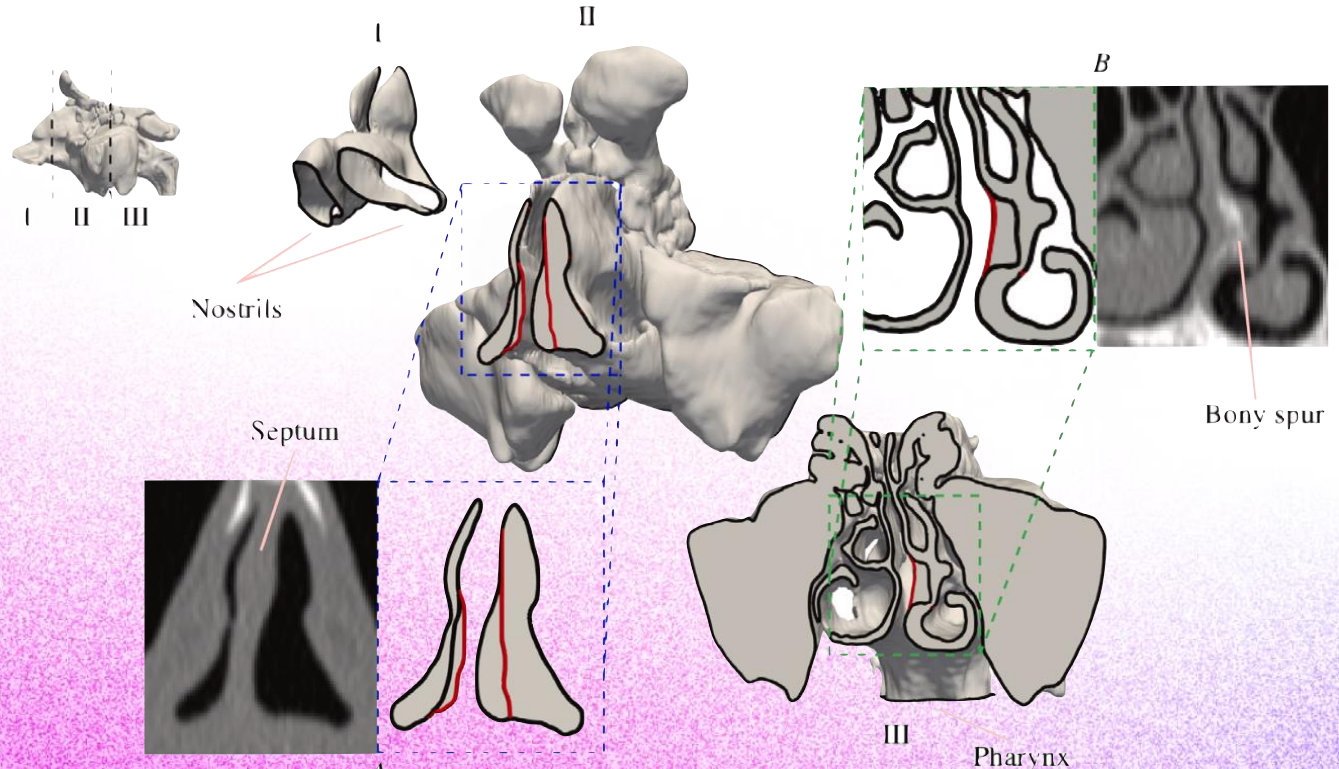
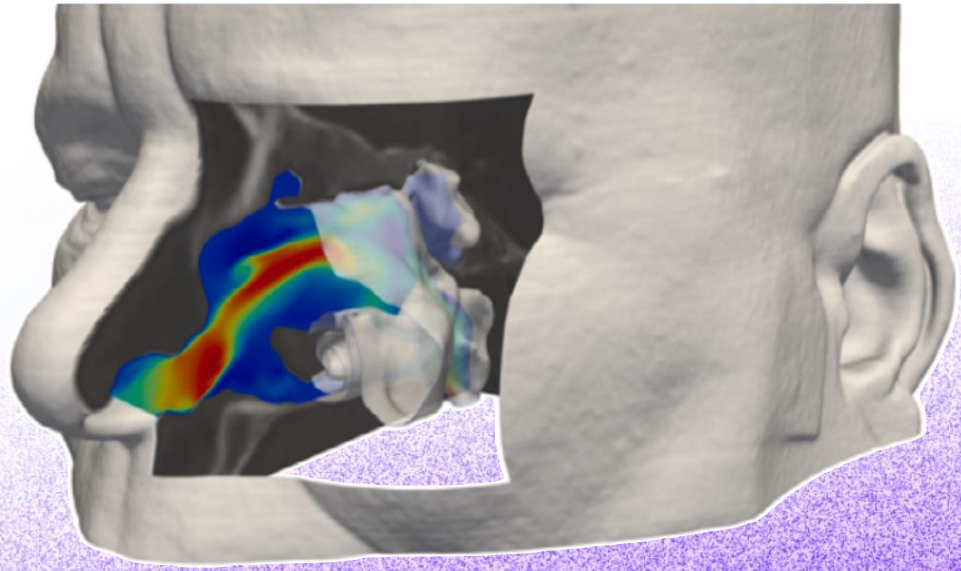
WP5P3

Personalized Medicine on Macroscopic Level:

Respiratory Flows and Infection Risk Analyses





WP5P3 Personalized Medicine on Macroscopic Level: Respiratory Flows and Infection Risk Analyses

T5.5 - AI-assisted automated CFD pipelines and acceleration of CFD computations

M1 01.03.2024 until M36 27.02.2027	JÜLICH Forschungszentrum RIKEN KOBE UNIVERSITY	**Acceleration and automation of respiratory flow CFD simulation pipelines through AI:** – Super-resolution with CNNs for upscaling of computer tomography data – Flow field initialization with physics-aware neural networks for simulation acceleration – Parallel training of neural networks with specifically tuned AI software and hardware components

M5.1	Several collaborative interactions in place such as visits and exchanges	M18 – 08.2025
R5.5	Intermediate report on scientific advancements in Personalized Medicine at the Macroscopic Level	M21 – 11.2025

T5.6 - AI-assisted surgery planning and risk assessment of exhaled infectious aerosols

M1 01.03.2024 until M36 27.02.2027	JÜLICH Forschungszentrum RIKEN KOBE UNIVERSITY	**AI-assisted surgery planning and waiting room scenario for risk assessment of viral infection** – Reinforcement learning algorithm for human airway geometry modification suggestions - Extension of objective function and action space for this RL algorithm - Waiting-room scenario with risk evaluation through viral particle tracking

M5.1	Several collaborative interactions in place such as visits and exchanges	M18 – 08.2025
R5.6	Final report on scientific advancements in Personalized Medicine at Macroscopic Level	M36 – 02.2027

WP5P3 Personalized Medicine on Macroscopic Level: Respiratory Flows and Infection Risk Analyses

- Monthly meetings with Japanese researchers to exchange progress of the Joint Laboratory for Extreme Scale Computing (JLESC) Project “Deep Neural Networks for CFD Simulations”

- Further online meetings to achieve the following:
  - Joint publication about physics-informed neural networks for flow predictions[1]
  - Joint publication about the decomposition of flow fields with machine learning[2]
  - Joint submissions to the Workshop on Advancements of Global Challenges Applications (AGCA), held in conjunction with the 15th International Conference on Parallel Processing and Applied Mathematics PPAM 2024[3,4]

[1]

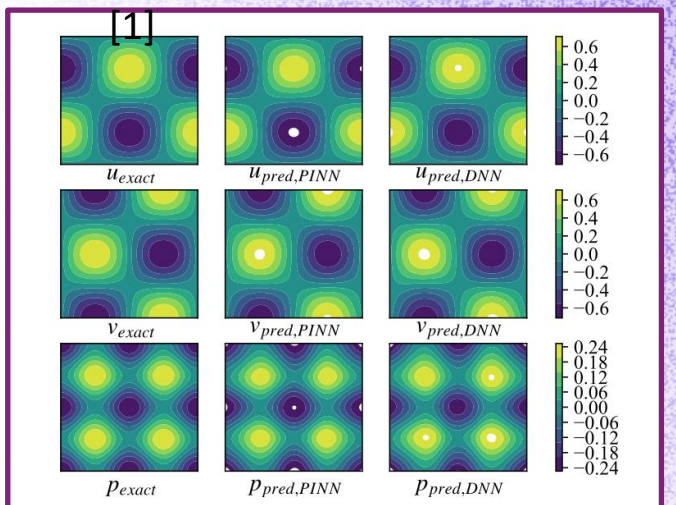


Fig. 18. Comparison of the prediction performance of the reduced PINN and DNN models for the two-dimensional Taylor–Green vortex at $t = 17$ s and $\mathcal{F} = 0.05$. The blank regions are predictions outside the range of the ground truth.

[2]

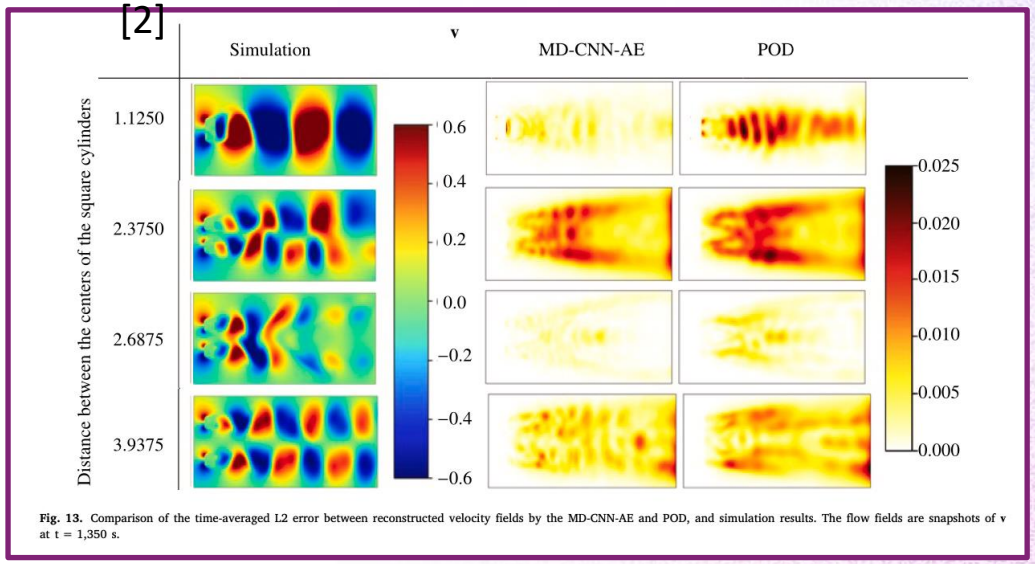


Fig. 13. Comparison of the time-averaged L2 error between reconstructed velocity fields by the MD-CNN-AE and POD, and simulation results. The flow fields are snapshots of v at t = 1,350 s.

[1] Rishabh Puri, Junya Onishi, **Mario Rüttgers**, Rakesh Sarma, **Makoto Tsubokura**, **Andreas Lintermann**: On the choice of physical constraints in artificial neural networks for predicting flow fields, Future Generation Computer Systems, Volume 161, 2024, doi:10.1016/j.future.2024.07.009.

[2] Aito Higashida, Kazuto Ando, **Mario Rüttgers**, **Andreas Lintermann**, **Makoto Tsubokura**: Robustness evaluation of large-scale machine learning-based reduced order models for reproducing flow fields, Future Generation Computer Systems, Volume 159, 2024: 10.1016/j.future.2024.05.005.

[3] **Mario Rüttgers**, Fabian Hübenthal, **Makoto Tsubokura**, **Andreas Lintermann**: Parallel reinforcement learning and Gaussian process regression for improved physics-based nasal surgery planning, AGCA workshop, PPAM conference, Ostrava, 2024.

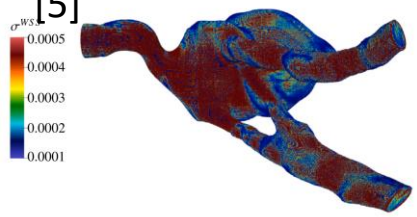
[4] **Makoto Tsubokura**, Rahul Bale, Alicia Murga, Kazuhide Ito, **Mario Rüttgers**, **Andreas Lintermann**: HPC-CFD based optimization of indoor environment to minimize airborne containments, AGCA workshop, PPAM conference, Ostrava, 2024.

WP5P3 Personalized Medicine on Macroscopic Level: Respiratory Flows and Infection Risk Analyses

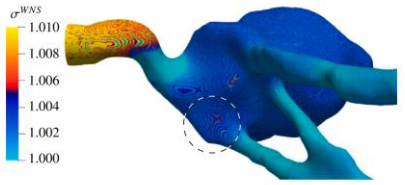
- Monthly meetings with Japanese researchers to exchange progress of the Joint Laboratory for Extreme Scale Computing (JLESC) Project “Deep Neural Networks for CFD Simulations”

- Recent publication on experimental-data-driven boundary conditions for LBM simulations[5] - this application can be extended for boundary conditions for respiratory flow simulations
- Another paper is currently in review[6] to advance the use of CFD in rhinology

[5]



(a) WSS for the simulation with the CY model for non-Newtonian fluid flow.



(b) WNS for the simulation with the CY model for non-Newtonian fluid flow.

[6]

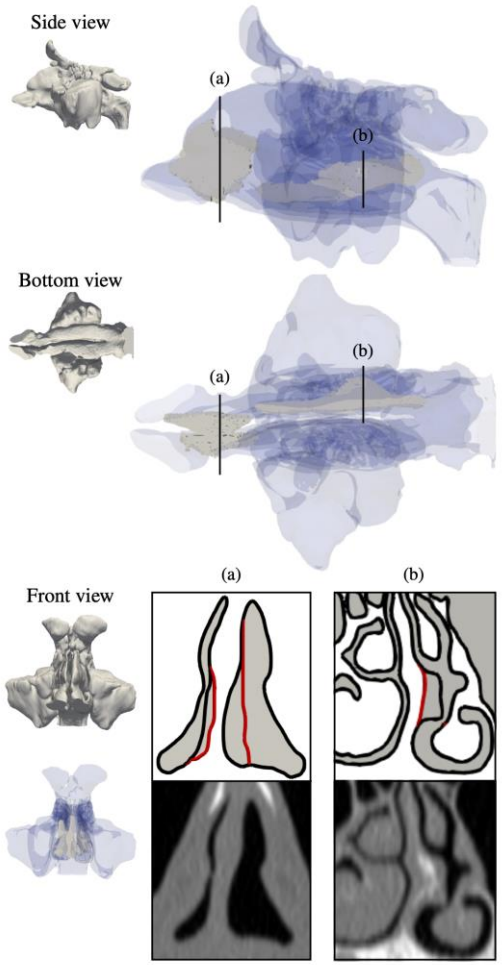


Figure 1: The nasal cavity of the first patient, suffering from a deviated septum and a bony spur (Case A), which was investigated in [11, 14, 17]. The bounds of a surgeon’s initial idea of the desired post-operative result are illustrated by the grey 3D regions inside of the transparent-blue representations of the nasal cavity. The close-ups (a) and (b) on the right side correspond to the lines depicted in the 3D images above. They illustrate boundaries at representative cross-sectional areas, which are juxtaposed to the corresponding pre-surgical CT images below. The black and red contours represent the boundaries of the pre-surgical structure and the geometry based on a surgeon’s initial idea of the desired post-operative result.

[5] Mario Rüttgers, Moritz Waldmann, Shota Ito, Carolin Wüstenhagen, Sven Grundmann, Martin Brede, and Andreas Lintermann, Patient-specific lattice-Boltzmann simulations with inflow conditions from magnetic resonance velocimetry measurements for analyzing cerebral aneurysms, Computers in Biology and Medicine, 187, 109794, 2025.
[6] Mario Rüttgers, Moritz Waldmann, Fabian Hübenthal, Klaus Vogt, Makoto Tsubokura, Sangseung Lee and Andreas Lintermann, Towards a widespread usage of computational fluid dynamics simulations for automated virtual nasal surgery planning - in review

WP5P3 Personalized Medicine on Macroscopic Level: Respiratory Flows and Infection Risk Analyses

Presenting the first HANAMI results at PPAM 2024


PPAM 2024
15th INTERNATIONAL CONFERENCE ON PARALLEL PROCESSING AND APPLIED MATHEMATICS

DIPLOMA

PPAM Best Paper Award

The International Conference on Parallel Processing and Applied Mathematics (PPAM) Best Paper Award is given upon recommendation of the PPAM Chairs and Program Committee in recognition of the research paper's quality, originality, and significance of the work in high performance computing.
The PPAM Best Paper was first awarded at PPAM 2019 in Bialystok.

PPAM 2024 Award for Workshop is bestowed to:

***Mario* Rüttgers**
Fabian Hübenthal
Makoto Tsubokura
Andreas Lintermann

„Parallel reinforcement learning and Gaussian process regression for improved physics-based nasal surgery planning"

CHAIRS OF PROGRAM COMMITTEE

Roman Wyrzykowski,
Ewa Deelman

Ostrava, Czech Republic, September 8-11, 2024

Makoto Tsubokura, Rahul Bale, Alicia Murga, Kazuhide Ito, **Mario Rüttgers**, **Andreas Lintermann**: HPC-CFD based optimization of indoor environment to minimize airborne containments, AGCA workshop, PPAM conference, Ostrava,

Mario Rüttgers, Fabian Hübenthal, **Makoto Tsubokura**, **Andreas Lintermann**: Parallel reinforcement learning and Gaussian process regression for improved physics-based nasal surgery planning,

WP5P3 Personalized Medicine on Macroscopic Level: Respiratory Flows and Infection Risk Analyses

Supercomputers access

- Access granted for WP5, P3 Japanese researchers to JURECA-DC through the VSR compute project ”Improved Diagnostics of Respiratory Flows Using a Lattice-Boltzmann Method and Machine Learning Techniques” – duration: 05.2024 until 04.2025 - **completed**
  - JURECA DC Module CPU: 1.76 million core-h
  - JURECA DC Module GPU: 2.60 million core-h
- Compute time extension (05.2025-04.2026) submitted on 17.02.2025, granted
  - JURECA DC Module CPU: 1.22 million core-h
  - JURECA DC Module GPU: 1.57 million core-h
- Development access will be requested for JUPITER (JEDI access already available)
- Access to FUGAKU: 1.50 million core-h

WP5P3 Personalized Medicine on Macroscopic Level: Respiratory Flows and Infection Risk Analyses

Codes relevant for WP5 P3		
Code	**Supercomputers**	**Stage**
m-AIA	JUWELS, JURECA-DC, JEDI, Hunter (HLRS)	Production
	Fugaku	Start
CUBE	Fugaku	Production
	JUWELS, JURECA-DC, JUPITER (planned)	Start

FZJ also participates in AI4HPC project, which provides a repository of useful AI models trained on CFD datasets.

This repository can also be used as a shared workspace to integrate the models and datasets generated by the Japanese researchers at RIKEN-CCS and Kobe University. They can also have unrestricted access to models and datasets generated at FZJ through HANAMI.

WP5P3 Personalized Medicine on Macroscopic Level: Respiratory Flows and Infection Risk Analyses

Proposals

- New proposal - Fund for the Promotion of Joint International Research (International Leading Research) category of the Grants-in-Aid for Scientific Research (KAKENHI)
  - PI: Makoto Tsubokura, RIKEN/R-CCS
  - Andreas Lintermann acts as an International Joint Researcher

Projects & visits

- Prof. Makoto Tsubokura visit the FZJ to discuss further collaboration on 03.03.2025
- HANAMI travelling grants
  - Visit from Aleksandr planned in 09.2025 - feasibility and other details to be discussed with Hanami organizing team.
- Codes
  - Discussing the portability of the *m-AIA* code on the Fugaku supercomputer
  - Running the developed tools on the Fugaku supercomputer
  - Effective work starting on 04.2025
- Negotiation of visiting researcher contract at R-CCS

WP6

HPC for future materials design

WP6 objectives and presentation

WP6 HPC for future materials design

- HPC to study and optimize various materials properties to develop sustainable energy technologies

- HPC enables new dimensions of materials design, increasing
  - complexity of the accessible systems and properties,
  - accuracy and improved approximations of the computational approaches

- Combination of HPC, high-throughput and materials informatics capacities,
  - Address major societal and technological challenges

- Strengthening the EU-Japan collaboration
  - Improving materials sustainability in applications of relevance for energy production and storage
  - Joint development efforts for extremely scalable libraries and innovative software that may enable future applications at the frontiers of knowledge
- Push the frontiers of in silico simulations of innovative materials for sustainable energy production and storage

- Share and advancing optimized codes developed in Europe and Japan
  - Interoperability and use on the most performing systems

- Develop numerical libraries capable of executing at scale

- Identify future challenges and opportunities for materials research in the evolving HPC ecosystem and in emerging technological trends

WP6 HPC for future materials design

Work package leaders

Elisa Molinari **Edoardo Di Napoli**

HANAMI members

HANAMI participants

- 2 projects within WP6, each project is divided in 3 tasks
  - WP6 – P1: Sustainable materials for photovoltaics and energy storage
  - WP6 – P2: Exascale Materials Science simulations through extremely scalable libraries and innovative software

WP6 HPC for future materials design

M6.1	All HANAMI code, workflows and databases developed in project available in public repositories or servers.	M18 – 08.2025	
M6.2	Snapshot of the major codes involved in the WP in the form of code releases addressing the code improvements accessible in publicly available repository	M36 – 02.2027	
R6.1	Report on the initial set up of the projects and the building and consolidating of the collaborations with the Japanese partners	M06 - 08.2024	**Delivered on time**
R6.2	First projects results and outlook on sustainability of EU-Japan collaboration with indication of prospective enlargement of collaborative partnership	M18 – 08.2025	
R6.3	Results of the projects and outlook on future activities.	M36 – 02.2027	

WP6 ongoing actions

WP6 – Project 1

Sustainable materials for photovoltaics and energy storage

Project 1 **Sustainable materials for photovoltaics and energy storage**

Giacomo Giorgi

Daniele Varsano

Maurizia Palummo

Koich Yamashita

Takahito Nakajima

T6.1 - Sustainable materials for photovoltaics		
M1 01.03.2024 until M36 27.02.2027	National Research Council of Italy RIKEN 横浜市立大学 YOKOHAMA CITY UNIVERSITY 東京大学 THE UNIVERSITY OF TOKYO	Characterize more sustainable materials for **perovskite-based solar cells (PSCs), in particular Pb-less and Pb-free PSCs**. Calculate the interface and GBs from first-principles combining such calculations with large-scale quantum chemistry ones to study their impact on the devices and to the assembling of the active interfaces in tandem cells to predict how the stress may alter the optoelectronic features of the final PSC. **Optimize the codes in the Japan and EuroHPC machines** for efficient calculation in large **relevant in perovskite-based solar cells with a particular effort in Distributed solver in large matrix Bethe-Salpeter equation.** . Yambo 富岳 NTChem

WP6 HPC for future materials design – **research team**

Pablo Ordejon

Deborah Prezzi

Stefan Blugel

Yoshitaka Tateyama

Minoru Otani

T6.2 - Electrochemistry and battery research from first principles

M1
01.03.2024

until

M36
27.02.2027

ICN2

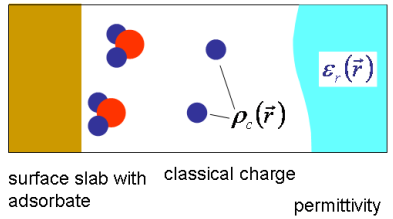
National Research Council of Italy

JÜLICH Forschungszentrum

NIMS 物質・材料研究機構

筑波大学 University of Tsukuba

The groups in Japan have employed DFT methods to electrochemical problems. Japan is advanced in the formulation of theoretical methods to study the electrified electrode-electrolyte interface
(Effective Screening Medium - ESM
by Otani and Sugino)



The EU team is expert in the development of DFT methods and their implementation on efficient codes (SIESTA). They have also developed methods to study the electrified interface based on alternative approaches (Non-Equillibrium Green's Functions).

siesta TM

The work in HANAMI aims to: (1) **implement the ESM method in SIESTA** , to improve the realism of the simulations by introducing a continuum approach for the electrolyte, and (2) **optimize the code in the Japan and EuroHPC machines** and **demonstrate efficient and relevant calculations of the electrified interface in battery materials**.

WP6 HPC for future materials design – **research team**

Michele Casula

Marco Cherubini

Kosuke Nakano

Abhishek Raghav

T6.3 - Hydrogen storage mechanisms from quantum Monte Carlo (QMC)		
M1 01.03.2024 until M36 27.02.2027	cnrs NIMS	Evaluate the **chemical binding energy of hydrogen-bonded systems** by employ the **TurboRVB code**, which implements efficient **quantum Monte Carlo (QMC)** algorithms and which also includes a built-in path integral molecular dynamics driver. *Main developers: Michele Casula (CNRS), Kosuke Nakano (NIMS)*
		Obtain highly accurate reaction barriers from QMC simulations including **nuclear quantum effects** from predictive calculations from first principles.
		Combine QMC with Machine Learning to develop fast and accurate potential energy surfaces, and enhance the portability of TurboRVB towards HPC machines thanks to an efficient **CPU/GPU parallelization**. Workflow manager: **TurboGenius**

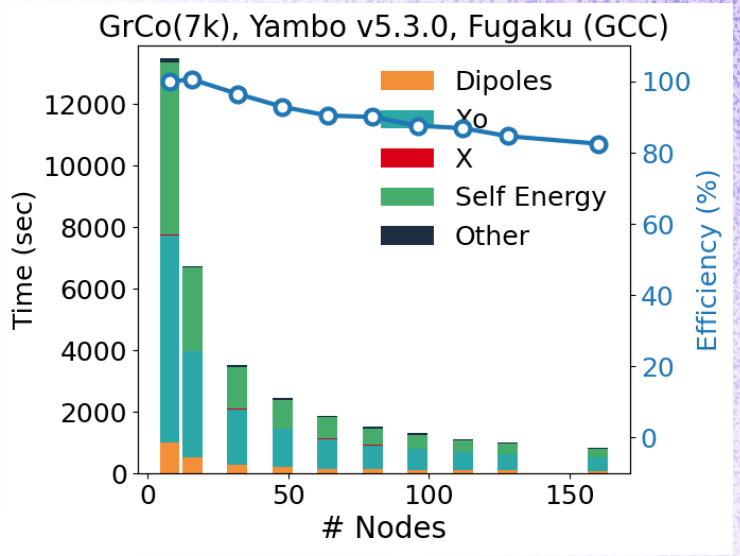
TurboRVB

Sustainable materials for photovoltaics and energy storage

- **Meetings with Japanese researchers**
  - Online and in person meetings (HLS1 Barcelona) discussing first steps for Pb-free photovoltaic project with Yokohama University Partner (K. Yamashita)
  - Online and in person meeting CNR- Riken Partner (W. Dawson) discussing reduced precision benchmark for Yambo and TurboRVB codes. Actions planned.
  - Joint publications with CNR-Japanese partners:
    1. *Unveiling the Origin of High Air Stability in PbS QD/ZnO Nanowire Heterojunction Solar Cells, submitted, ACS Applied Energy Materials*, ***Giacomo Giorgi***, *Takaya Kubo, et al.*
    2. *Hydrogen liquid-liquid transition from first principles and machine learning, submitted to PRB, arXiv preprint arXiv:2502.02447, G. Tenti, Bastian Jäckl,* ***Kosuke Nakano****, Matthias Rupp,* ***Michele Casula***
    3. *Planned Book Project: "Computational Modeling for Advanced Photovoltaics: Materials, Interfaces, and Phenomena for Beyond-Silicon Solar Cells" (Elsevier) as part of the "Theoretical and Computational Chemistry" book series. Edited by* ***Giacomo Giorgi*** *(University of Perugia), Sergei Manzhos (Institute of Science Tokyo), and others.*
  - Planning of a WP6 workshop to be held in Paris. Additional funding granted from CECAM-FR node – organization almost finalized, dates are released on the HANAMI website
  - In person meeting (HLS1 Barcelona, Jan 14th 2025) discussing details of the implementation of ESM in SIESTA, with Tsukuba University Partner (M. Otani)
  - Periodic zoom meetings between the ICN2 team and Tsukuba University Partner (M. Otani) on the implementation of ESM in SIESTA.
  - TurboRVB: weekly zoom meetings + Kosuke Nakano (NIMS) visit to Paris (Sorbonne U, CNRS) in September 1-8 2024 and in January 27-30 2025

Sustainable materials for photovoltaics and energy storage

Access in Supercomputers in Japan



- **Yambo Trial Access** Project, project Yambo Scale: hp240326 through HPCI access

  Duration: 09.2024 for 6 months. Maximum of computing hours: 100000 node-hours
  - Deployment and benchmarking of the Yambo code have been conducted.
  - A scaling benchmark using GCC compilation demonstrated good scalability.
  - Additional benchmarks with Fujitsu compilation are ongoing.
  - A report, including the compilation recipe and scaling benchmarks, is in preparation.

- **Fugaku Project Period-A of FY2025** – "Exascale and sustainable materials simulations through extremely scalable libraries and innovative software" was submitted and recently accepted; project number hp250100 through HPCI access

  Duration: 1 year starting April 1st 2025. Computing hours awarded: 6 Million node-hours (PI E. Di Napoli)

- **TurboRVB Regular Access Project**, project number hp240033 through HPCI access

  Duration: FY2024 (01.04.2024 - 31.03.2025) Maximum of computing hours: 5M nh

  Goal: Development of accurate QMC strategies to generate accurate training sets for machine learning

- **TurboRVB Regular Access Project,** project number hp250031 through HPCI access

  Duration: FY2025 (01.04.2025 - 31.03.2026)

  Goal: First-principles diffusion Monte Carlo calculations with TurboRVB beyond the Coupled Cluster accuracy.

Sustainable materials for photovoltaics and energy storage

Access in Supercomputers in Europe

- **TurboRVB Regular Access Project,** project number A0170906493 through GENCI access

Duration: 01.11.2024 - 31.10.2025. Maximum of computing hours: Rome TGCC (6.5M core hours), SkyLake TGCC (1M core hours), Jean-Zay IDRIS GPU V100 partition (0.72M GPU hours), Jean-Zay IDRIS CPU partition (0.48M CPU hours)

- **Yambo: ISCRA-B project Proposal** ID: IsB30_EISD 1.6M core hours on LEONARDO BOOSTER (CINECA, Italy). From 01/01/2025 to 01/01/2026

- **Siesta : Access to 16 out of 17 available EuroHPC JU partitions** (benchmark access to 15 partitions, development access to Deucalion ARM, regular access to VEGA CPU). Participation in JUREAP.

Access granted to MareNostrum5 (BSC, Spain) for 4M core hours from 1/3/25 to 30/6/25

GENCI
HPC at the service of knowledge

TGCC
Très Grand Centre de calcul du CEA

idris

WP6P1 Sustainable materials for photovoltaics and energy storage

- **HANAMI travelling grant** requested on 06.2024
  - Visit from researcher (Giorgi, Varsano, Borghesi) in 06-07.2025, 2-4 weeks; visited laboratory: Yamashita Lab (Yokohama, JP).
  - Visit of CNRS team (Casula, Raghav, Cherubini) in 04.2025, 2 weeks; visited laboratory: NIMS (Tsukuba, JP).
  - Two visits of ICN2 postdoctoral researcher to Otani group (Tsukuba, JP) in 03/25 and 01/26, each of them 1 month

- **Workshop** organization around WP6 topics involving both European and Japanese community. (Fall 2025). Extra funding from CECAM granted.
- **Action on codes :**
- Yambo
  - Porting and benchmark campaign on Fugaku supercomputer (completed with GCC compilation in Jan. 2025, ongoing with Fujitsu compilation)
  - Exploration of performance of different solvers in both European and Japanese machines (slepc, magma, ChASE)
  - Exploration of precision reduction in collaboration with RIKEN (started in Feb. 2026)
- TurboRVB
  - Portability of workflow manager TurboGenius across different (European and Japanese) HPC platforms
  - Exploration of different machine learning schemes for QMC-derived interatomic potentials
- SIESTA
  - Porting of ESM to the most recent version of SIESTA (version 5).
  - Porting, benchmarking and deployment of SIESTA 5 in EuroHPC systems with the same architecture as FUGAKU (eg. Deucalion CPU ARM).
  - Porting, benchmarking and deployment of SIESTA 5 in FUGAKU.

WP6P1 Sustainable materials for photovoltaics and energy storage

Recruitment:

- Task 6,1: Hired 2 Years Postdoc Position at CNR Dr. Costanza Borghesi.
  Theme: Photovoltaic application and enabling Yambo code to solve large excitonic matrixes
- Task 6.2: Hired 2 Years Postdoc (Dr. Nils Wittemeier) at ICN2. Start date: Oct 1, 2024.
  Theme: “Implementation of the EMS method in SIESTA”
- Task 6.3: 2 Postdoc Positions at CNRS started in May 2024 and ending in July 2025
  Theme postdoc 1: development of QMC data generation techniques adapted to the training of atomistic potentials by machine learning

  Theme postdoc 2: development of innovative techniques to compute lattice vibrations in hydrogen-rich compounds, based on machine learning interatomic potential built on top of QMC data.

Costanza Borghesi (CNR)

Nils Wittemeier (ICN2)

Marco Cherubini

Abhishek Raghav

WP6 Project 2

Exascale Materials Science simulations through extremely scalable libraries and innovative software

WP6 HPC for future materials design – research team

Edoardo Di Napoli

Toshiyuki Imamura

Luigi Genovese

Kengo Nagajima

William Dawson

Alessandro Pecchia

T6.4 - Numerical linear algebra framework for Materials Science

M1 01.03.2024 until M36 27.02.2027	JÜLICH Forschungszentrum	Standard framework for large-scale numerical linear algebra libraries development
	RIKEN cea	Provides a common platform for developers and users to access and utilize various numerical libraries and data structures
	National Research Council of Italy	Promotes interoperability and collaboration among the different supercomputing centersand research groups making up the EU-Japan landscape;
	東京大学 THE UNIVERSITY OF TOKYO	Enables researchers to easily benchmark and evaluate the performance of different parallel algorithms

WP6 HPC for future materials design – research team

Alessandro Pecchia

Takahito Nakajima

Tetsuya Sakurai

Taisuke Ozaki

Edoardo Di Napoli

Luigi Genovese

T6.5 - Non-equilibrium charge-carrier dynamics in 2d-materials		
M1 01.03.2024 until M36 27.02.2027	JÜLICH Forschungszentrum	Development of parallelNEGF & interfacing BigDFT Massively parallel solver with electron-phonon and electron-photon interactions
	RIKEN cea	Implement a framework for the representation of block sparse (with dense blocks) data operating close to peak memory bandwidth and tailored to accelerated platforms.
	National Research Council of Italy	Integrate both data framework and abstraction interface in MS code such as BigDFT and libNEGF.

WP6 HPC for future materials design – research team

Luigi Genovese

Takahito Nakajima

Sergeij Manzhos

Edoardo Di Napoli

Alessandro Pecchia

T6.6 - Enhancing Materials Science scalability through innovative block sparse libraries		
M1 01.03.2024 until M36 27.02.2027	cea	Extend the scaling fo BigDFT by progressively combining the current features of the code with ongoing developments in tasks 6.4
	RIKEN	Combine multiple numerical methods featuring a hierarchy of implementation that can be automatically adapted to current and feature supercomputing platforms.
		Enhance the capabilities of the simulation software and will extend the scope of linear-scaling electronic structure methods and quantum transport to other computer codes and formalisms
	National Research Council of Italy	Extend the block matrix representation of NTpoly in the dense format of DBCSR and include the Fermi Operator Expansion (FOE) approach in the new library which would employ block sparse DBCSR representation to benefit from GPU acceleration
	JÜLICH Forschungszentrum	Apply the Kernel Polynomial Methods on-top of the FOE approach to further reduce the number of Chebyshev polynomials to be calculated.

WP6P2 Exascale Materials Science simulations through extremely scalable libraries and innovative software

- Regular meetings with Japanese researchers
  - Monthly exchanges b/w FZJ and RIKEN on ChASE, EigenExa and the ELSI platform
  - Access to Gitlab based repositories for the exchange of information through the creation of Gitlab issues and merging requests
  - Exchange of additional messages and information through a Slack workspace.
  - Weekly meeting bw CEA-RIKEN in the framework of BigDFT/CheSS/NTpoly developments
  - New PhD student in collaboration with Tokyo University on efficient usage of BigDFT basis sets

slack

zoom

GitLab

WP6P2 Exascale Materials Science simulations through extremely scalable libraries and innovative software

Meetings and workshops with Japanese researchers

- Workshop in Forschungszentrum Juelich, Germany – March 13-15, 2024
  Participants : FZJ and RIKEN-CCS
- Working visit in Kobe (11.2023) by L. Genovese and of W. Dawson in Grenoble (05.2024) on the topic ‘HPC Workflows in Large scale Calculations’
- Visit of W. Dawson in Grenoble for 3 weeks in November 2024 – leverage action (grant received by the French embassy)
- Visit of Dr. A. Pecchia to Riken 20th April - 2nd May 2025
- Visit of Dr. Imamura to Forschungszentrum Juelich from 11.02 to 13.02.2025
- WP6 workshop to be held in Paris. Additional funding granted from CECAM-FR node.

cea

JÜLICH Forschungszentrum

RIKEN

WP6P2 Exascale Materials Science simulations through extremely scalable libraries and innovative software

Supercomputers access in Japan

- Access granted for FZJ team (for use with ChASE and EigenExa) to Fugaku through HPCI access – duration: 10.2023 until 09.2024
  - Maximum of computing hours: 3,200,000 node-h
- Access granted to FZJ team (for use with ChASE and libNEGF) to Wisteria through JHPCN – duration 05.2024 until 04.2025
- Access granted to CEA team (for use with BigDFT and Genesis) to Wisteria through JHPCN – duration 05.2024 until 04.2025
- Wisteria workflow calculations designed and running.
- Access granted to FUGAKU thanks to successful proposal on HPCI PA-FY2025
  - 1st April 2025 - 31st March 2026 - Granted computing hours: 5,960,088 node-h

Supercomputers access in Europe

- Access to be granted for WP6 P2 Japanese researchers to JUWELS and JUPITER through bilateral MoU FZJ and RIKEN/R-CCS
- Access granted to Leonardo for benchmark purposes for BigDFT and CheSS
- Access granted on LUMI for development project around the BigDFT GPU acceleration.

Exascale Materials Science simulations through extremely scalable libraries and innovative software

Recruitment:

- Task 6,4: Hired 2 Years Postdoc Position at Forschungszentrum Juelich—Juelich Supercomputing Centre. **Dr. Clement Richefort**.

  Theme: Integrate ChASE with the Yambo code and further develop ChASE to solve pseudo-Hermitian eigenproblems. Develop a parallel framework for the seamless integration of Material Science codes with Numerical linear algebra libraries.

- Task 6,5: Position awarded for a 2 Years Post Doc Position at CNR-ISMN (Interview completed on 14/02/2025).

  Theme: Perform transport simulations of 2D MoS_2/WS_2 bilayers for electronics and photovoltaic properties, probing especially the role of S-vacancies.

THANK YOU!

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EuroHPC Joint Undertaking

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